JLAB-THY-12-1659

The coupled-channel and three-particle system on a torus

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(Dated: November 6, 2012)

Based on the Hamiltonian formalism approach, a generalized Lüscher's formula for two particle scattering in both the elastic and coupled-channel cases in moving frames is derived from a relativistic Lippmann-Schwinger equation. Some strategies for extracting the phase shifts and inelasticity of a coupled-channel system from the finite-volume spectrum are discussed. Within the same framework, we extend our discussion to a three-particle system. A set of equations which relate the discrete finite-volume energies to the scattering amplitudes are derived under the approximation of the isobar model. These formalisms will, in the near future, be used to extract information about hadron scattering from lattice QCD computations.

PACS numbers: 12.38.Gc, 11.80.Gw, 11.80.Jy, 13.75.Lb
Keywords:

I. INTRODUCTION

Hadron spectroscopy in lattice QCD is entering a new era, in particular, recent developments in the application of variational methods [1–3] to large bases of hadron interpolating fields have made the extraction of the excited spectrum of hadronic states a realistic possibility (see e.g. [4–6]). Since excited hadrons appear as resonances in the continuous distribution of multi-hadron scattering states, to study hadron spectroscopy one requires evaluation of scattering amplitudes, but because lattice QCD is formulated in Euclidean space, we do not have direct access to these [7]. Fortunately, in a finite volume, interactions between particles as they evolve from the *in* to the *out* states lead to discrete changes in a free particle's energy that can be related to the scattering amplitude [8].

Various extensions to the framework derived by Lüscher in [8] have been proposed which allow for evaluation outside the center-of-mass frame [9–13], and to include the coupled-channel effects that can appear above the inelastic threshold [14–18]. The original approach and its extensions to describe the moving center-of-mass frame have been quite successfully used by the lattice community to extract elastic hadron-hadron scattering phase shifts[6, 19–25].

In this work, we discuss a generalization of Lüscher's method for relativistic scattering in terms of a Hamiltonian where the specific interactions considered are based on a relativistic particle exchange model. We apply the technique to a two-channel system and a generalized Lüscher's equation for scattering in a moving frame is derived based on the relativistic Lippmann-Schwinger equation. The coupled-channel system has been considered previously, [14, 15, 17, 18], and our result agrees with the form derived in a non-relativistic formalism in [14]. A novelty of the present work is to discuss practical strategies for extraction of scattering amplitude parameters (phase shifts and inelasticities) from lattice simulations of a coupled-channel system. These strategies are demonstrated using an explicit toy model of resonant two-channel scattering.

We also discuss the three-particle system, considering the finite-volume representation of the isobar model [26, 27] in which interactions in the three-particle system are approximated by two-body scattering. We derive expressions which relate finite-volume energy shifts to isobar-model scattering amplitudes.

The paper is organized as follows. A discussion of the elastic scattering in a finite-volume is given in Section II, with the extension to the coupled channel system in Section III. Strategies for extracting scattering amplitudes from measured discrete finite-volume spectra are presented in Section IV. In Section V we discuss the three-particle system, with summary and outlook given in Section VI.

II. FINITE-VOLUME ELASTIC SCATTERING IN A HAMILTONIAN FRAMEWORK

In this section we present relativistic two-particle scattering on a torus using the Hamiltonian formalism developed in [28, 29]. In particular we consider a complex scalar field, Φ, describing a charged boson, $\phi^{\pm}$, of mass m, and its interactions with a neutral boson, θ, which acts as a force carrier and is described by a real scalar field, Θ. We first derive the Lüscher formula describing the finite-volume spectrum of the asymptotic two-

particle, $\phi^+\phi^-$ state,

$$\det\left[\delta_{JM,J'M'}\cot\delta_J(k) - \mathcal{M}^{(\mathbf{Q})}_{JM,J'M'}(k)\right] = 0,$$

where the volume and scattering-frame dependent matrix element $\mathcal{M}^{(\mathbf{Q})}_{JM,J'M'}$ is defined in Eq.(B1) and (B3), and the center-of-mass frame scattering momentum, k, is related to the energy by $\sqrt{s/4-m^2}$. The model corresponds to a Lagrangian density,

$$\mathcal{L} = \partial_\mu\Phi^*\partial^\mu\Phi - m^2\Phi^*\Phi + \tfrac{1}{2}\partial_\mu\Theta\partial^\mu\Theta - \tfrac{1}{2}\mu^2\Theta^2 - g\Theta\Phi^*\Phi, \tag{1}$$

from which the Hamiltonian can be derived following the canonical procedure of instant-time quantization (see Appendix A) [30]. Taking matrix elements of the Hamiltonian in an infinite basis of Fock states spanned by any number of ϕ and θ bosons one can obtain a Schrödinger equation $\hat{H}|\Psi\rangle = E|\Psi\rangle$ for the eigenstates of the theory. Assuming $\mu \gg m$, in describing low-energy ϕ-boson scattering we can truncate the Fock space to include up to one θ-boson in the intermediate state, which reduces the Schrödinger equation to

$$\begin{bmatrix} H_{22} & H_{23} \\ H_{32} & H_{33}\end{bmatrix}\begin{bmatrix}|\phi^+\phi^-\rangle \\ |\phi^+\phi^-\theta\rangle\end{bmatrix} \;=\; E\begin{bmatrix}|\phi^+\phi^-\rangle \\ |\phi^+\phi^-\theta\rangle\end{bmatrix}. \tag{2}$$

The three-particle sector can be formally eliminated, resulting in an effective two-body equation,

$$(E - H_{22})|\phi^+\phi^-\rangle = H_{23}\frac{1}{E-H_{33}}H_{32}|\phi^+\phi^-\rangle. \tag{3}$$

A. Two-particle scattering in an infinite volume

Before considering two-particle states on a torus, we will first review the scattering problem in infinite-volume, with further details given in Appendix A. After eliminating the three-particle states $|\phi^+\phi^-\theta\rangle$ from the coupled system (*cf* Eq.(2)) we are left with an equation for the center-of-mass frame momentum-space wavefunction, $\varphi_{JM}(\mathbf{q})$, which is a product of a radial wavefunction depending on the magnitude of the relative 3-momentum, $q = |\mathbf{q}|$, and the spherical harmonic of definite angular momentum, (J, M),

$$\varphi_{JM}(\mathbf{q}) = \frac{1}{\sqrt{s} - 2\sqrt{\mathbf{q}^2+m^2}}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\,V(\mathbf{q},\mathbf{k})\,\varphi_{JM}(\mathbf{k}). \tag{4}$$

Here, $E = \sqrt{s}$ is the energy of the two-particle system in the center-of-mass frame. The non-local potential, $V(\mathbf{q},\mathbf{k})$, induced by θ-exchange is given explicitly in Eq. (A1). Expressing this equation in coordinate space via a Fourier transform gives

$$\psi_{JM}(\mathbf{r}) = \int d^3\mathbf{r}'\,G_0(\mathbf{r}-\mathbf{r}';\sqrt{s})\int d^3\mathbf{z}\,\tilde{V}(\mathbf{r}',-\mathbf{z})\,\psi_{JM}(\mathbf{z}), \tag{5}$$

where the free Green's function is given by

$$G_0(\mathbf{r}-\mathbf{r}';\sqrt{s}) = \int\frac{d^3\mathbf{q}}{(2\pi)^3}\,\frac{e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}}{\sqrt{s}-2\sqrt{\mathbf{q}^2-m^2}}. \tag{6}$$

The wavefunction satisfies a relativistic Schrödinger equation,

$$\left(\sqrt{s} - 2\sqrt{-\nabla^2+m^2}\right)\psi_{JM}(\mathbf{r}) = \int d^3\mathbf{z}\,\tilde{V}(\mathbf{r},-\mathbf{z})\,\psi_{JM}(\mathbf{z}). \tag{7}$$

While Eq.(5) was derived in the context of a particular model, our subsequent derivation only requires the general form of the relativistic Lippmann-Schwinger equation. The asymptotic component of the two-body wavefunction relevant to scattering is given by the large distance behavior of the Green's function. Evaluating the integral in Eq.(6) (*cf.* Appendix A), we find

$$G_0(\mathbf{r};\sqrt{s}=2\sqrt{k^2+m^2}) = \\ -\frac{\sqrt{s}}{2}\,\frac{e^{ikr}}{4\pi r} - \frac{1}{r}\int_m^\infty\frac{\rho\,d\rho}{(2\pi)^2}\,\sqrt{\rho^2-m^2}\,\frac{e^{-\rho r}}{k^2+\rho^2}, \tag{8}$$

with the first term on the right hand side dominating as $r\to\infty$. For a potential $\tilde{V}$ which falls at large separations, the solution to Eq (7) outside the range of the interaction is given by

$$\psi_{JM}(\mathbf{r}) \to \frac{\sqrt{s}}{2m}i^J\,Y_{JM}(\hat{\mathbf{r}})\left[4\pi\,j_J(kr) + ik\,f_J(k)\,h^+_J(kr)\right], \tag{9}$$

where $f_J(k)$ is the partial wave scattering amplitude,

$$f_J(k) = -\frac{m}{i^J}\int d^3\mathbf{r}'d^3\mathbf{z}\,j_J(kr')\,Y^*_{JM}(\hat{\mathbf{r}}')\,\tilde{V}(\mathbf{r}',-\mathbf{z})\,\psi_{JM}(\mathbf{z}), \tag{10}$$

which up to the inelastic threshold can be parameterized in terms of a single real momentum-dependent parameter, the scattering phase-shift, $\delta_J(k)$, as

$$f_J(k) = \frac{4\pi}{k}e^{i\delta_J}\sin\delta_J.$$

B. Two-particle scattering on a torus

Now we consider the theory in a cubic box of volume $V = L^3$, with periodic boundary conditions. In Eq. (5) we split the integral over $\mathbf{r}'$ into a sum of integrals over a set of boxes labelled by the integers $\mathbf{n}$ representing the location of one of its corners,

$$\psi^{(L)}_{JM}(\mathbf{r}) = \sum_{\mathbf{n}\in\mathbb{Z}^3}\int_{L^3}d^3\mathbf{r}'\,G_0(\mathbf{r}-\mathbf{r}'-\mathbf{n}L;\sqrt{s}) \\ \times\int d^3\mathbf{z}'\,\tilde{V}(\mathbf{r}'+\mathbf{n}L,-\mathbf{z}'-\mathbf{n}L)\,\psi^{(L)}_{JM}(\mathbf{z}'+\mathbf{n}L). \tag{11}$$

In general we can make the wavefunctions periodic up to a phase,

$$\psi^{(L)}_{JM}(\mathbf{z}+\mathbf{n}L) = e^{i\mathbf{Q}\cdot\mathbf{n}L}\psi^{(L)}_{JM}(\mathbf{z}),$$

where the Bloch wave-vector, $\mathbf{Q}$, is related to the total momentum of the two-particle system [9] by $\mathbf{P} = 2\gamma\,\mathbf{Q}$. $\gamma = \sqrt{s+\mathbf{P}^2}/\sqrt{s}$ is the Lorentz contraction factor that reduces the effective size of the box in the direction parallel to $\mathbf{P}$. Using the periodicity of the potential, $\tilde{V}(\mathbf{r}'+\mathbf{n}L, -\mathbf{z}'-\mathbf{n}L) = \tilde{V}(\mathbf{r}', -\mathbf{z}')$, and the boundary condition on the wavefunction, we have

$$\psi^{(L,\mathbf{Q})}_{JM}(\mathbf{r}) = \int_{L^3} d^3\mathbf{r}'\, G_{\mathbf{Q}}(\mathbf{r}-\mathbf{r}';\sqrt{s}) \times \int d^3\mathbf{z}\,\tilde{V}(\mathbf{r}',-\mathbf{z})\,\psi^{(L,\mathbf{Q})}_{JM}(\mathbf{z}),$$

which is analogous to the infinite-volume equation, but with the Green's function given by

$$G_{\mathbf{Q}}(\mathbf{r}-\mathbf{r}';\sqrt{s}) = \sum_{\mathbf{n}\in\mathbb{Z}^3} G_0(\mathbf{r}-\mathbf{r}'-\mathbf{n}L;\sqrt{s})\, e^{i\mathbf{Q}\cdot\mathbf{n}L}.$$

Using the Poisson summation formula, $(2\pi)^{-3}\sum_{\mathbf{n}\in\mathbb{Z}^3} e^{i\mathbf{Q}\cdot\mathbf{n}L} = L^{-3}\sum_{\mathbf{n}\in\mathbb{Z}^3}\delta\left(\mathbf{Q}+\frac{2\pi}{L}\mathbf{n}\right)$, we obtain

$$G_{\mathbf{Q}}(\mathbf{r}-\mathbf{r}';\sqrt{s}) = \frac{1}{L^3}\sum_{\mathbf{q}\in P_{\mathbf{Q}}} \frac{e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}}{\sqrt{s}-2\sqrt{\mathbf{q}^2+m^2}} \to \frac{\sqrt{s}}{2}\frac{1}{L^3}\sum_{\mathbf{q}\in P_{\mathbf{Q}}}\frac{e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}}{k^2-\mathbf{q}^2},$$

where $P_{\mathbf{Q}} = \{\mathbf{q}\in\mathbb{R}^3 |\, \mathbf{q} = \frac{2\pi}{L}\mathbf{n}+\mathbf{Q},\ \text{for } \mathbf{n}\in\mathbb{Z}^3\}$, and where we have retained only the leading term in the limit $L \gg |\mathbf{r}-\mathbf{r}'| \gg m^{-1}$. Finally, expanding Eq.(11) for $r \gg r'$ and using the definition of the scattering amplitude, Eq. (10) we can express the wavefunction as

$$\psi^{(L,\mathbf{Q})}_{JM}(\mathbf{r}) \to \frac{\sqrt{s}}{2m}(-k)\, i^J f_J(k)\sum_{J'M'} Y_{J'M'}(\hat{\mathbf{r}}) \times \left[\delta_{JM,J'M'}\, n_{J'}(kr) - \mathcal{M}^{(\mathbf{Q})}_{JM,J'M'}(k)\, j_{J'}(kr)\right]. \tag{12}$$

The residual sum over all angular momenta reflects the broken rotational invariance induced by the finite cubic volume, with the volume-dependent matrix elements $\mathcal{M}$ given in Appendix B. In the infinite-volume case, the most general solution of the relativistic Schrödinger equation, Eq.(7), outside the range of the potential is $\sum_{JM} c_{JM}\,\psi_{JM}(\mathbf{r})$ for $\psi_{JM}(\mathbf{r})$ given by Eq. (9). Correspondingly in finite-volume, the most general solution is given by $\sum_{JM} c_{JM}\,\psi^{(L,\mathbf{Q})}_{JM}(\mathbf{r})$ for $\psi^{(L,\mathbf{Q})}_{JM}(\mathbf{r})$ given by Eq.(12). Matching the two wavefunctions at a fixed r, larger than the range of the interaction, we obtain

$$\sum_{JM} c_{JM} Y_{JM}(\hat{\mathbf{r}})\, i^J\left[4\pi\, j_J(kr) + ik\, f_J(kr)\, h^+_J(kr)\right] = -\sum_{JM,J'M'} c_{JM}\, i^J k\, f_J(k)\, Y_{J'M'}(\hat{\mathbf{r}}) \times \left[\delta_{JM,J'M'}\, n_{J'}(kr) - \mathcal{M}^{(\mathbf{Q})}_{JM,J'M'}(k)\, j_{J'}(kr)\right],$$

which has a non-trivial, $c_{JM}\neq 0$, solution provided

$$\det\left[\delta_{JM,J'M'}\,\cot\delta_J(k) - \mathcal{M}^{(\mathbf{Q})}_{JM,J'M'}(k)\right] = 0. \tag{13}$$

This condition expresses the relationship between the asymptotic behavior of the two-particle wavefunction on a torus, expressed through the matrix elements $\mathcal{M}^{(\mathbf{Q})}_{JM,J'M'}$, and the effect of the interaction on the wavefunction determined by the phase shifts, δ_J. In practice for a given set of elastic phase-shifts, $\delta_J(k)$, it determines a discrete spectrum of states in a finite volume.

The analysis presented here can be generalized to an arbitrary shaped box. In general the three edges of box are spanned by three arbitrary vectors $\mathbf{L}_{1,2,3}$. The volume of the cube L^3 is replaced by $(\mathbf{L}_1\times\mathbf{L}_2)\cdot\mathbf{L}_3$ and the vector $\mathbf{n}L$ by $\sum_{i=1,2,3} n_i\mathbf{L}_i, n_i\in\mathbb{Z}$. Finally the momentum $\mathbf{q} = 2\pi\mathbf{n}/L, \mathbf{n}\in\mathbb{Z}^3$ is replaced by generalized momentum $2\pi\sum_{i=1,2,3} n_i(\mathbf{L}_j\times\mathbf{L}_k)/|(\mathbf{L}_1\times\mathbf{L}_2)\cdot\mathbf{L}_3|, n_i\in\mathbb{Z}$, where indices (i,j,k) follow the cyclic permutation. Such a generalization has to be considered when using the moving center-of-mass frame since the symmetric shape of a cubic box in the rest frame is deformed due to Lorentz contraction [9]. In this case if $\mathbf{P} = 2\pi\mathbf{d}/L, \mathbf{d}\in\mathbb{Z}^3$, is the center-of-mass momentum, the volume of the box becomes γL^3, and the vectors $\mathbf{n}L$ and $2\pi\mathbf{n}/L$ are replaced by $\gamma\mathbf{n}L$ and $2\pi\gamma^{-1}\mathbf{n}/L$, respectively (using the notation defined in [9]). With these substitutions and the relation $\mathbf{P} = 2\gamma\mathbf{Q}$, our definition of the matrix elements $\mathcal{M}^{(\mathbf{Q})}_{JM,J'M'}$ becomes identical to the matrix elements $M^{\mathbf{d}}_{lm,l'm'}$ in Eq.(89) of [9].

Typically, as discussed in [8], for the low-energy region that we are interested in, higher partial waves become progressively smaller and can be ignored, so that the partial wave basis can be truncated at a certain maximal angular momentum $J_{\max}$. For a finite-volume with cubic boundaries, the continuous rotation symmetry is reduced to the little group of allowed cubic rotations that leave the centre-of-mass momentum invariant - the matrices in Eq.(13) become block-diagonal if subduced according to the irreducible representations of these little groups. Details of subduction in general moving frames can be found in [31].

III. COUPLED CHANNEL SCATTERING IN FINITE VOLUME

We extend the model of the previous section to include additional two-particle asymptotic states, by adding another species of charged bosons, $\sigma^{\pm}$, which also couples

to the force carrier, θ, into the Lagrangian. We can obtain coupled equations for the two-particle states, $|\phi^+\phi^-\rangle$ and $|\sigma^+\sigma^-\rangle$, by eliminating states featuring three or more particles and obtain a two-channel Schrödinger equation,

$$\begin{aligned}
|\phi^+\phi^-\rangle &= \frac{1}{E - H^{(0)}_\phi}\left[V_{\phi\phi}|\phi^+\phi^-\rangle + V_{\phi\sigma}|\sigma^+\sigma^-\rangle\right],\\
|\sigma^+\sigma^-\rangle &= \frac{1}{E - H^{(0)}_\sigma}\left[V_{\sigma\phi}|\phi^+\phi^-\rangle + V_{\sigma\sigma}|\sigma^+\sigma^-\rangle\right], \quad (14)
\end{aligned}$$

where $H^{(0)}_\phi$, $H^{(0)}_\sigma$ are the one-particle operators and $V_{\phi\phi}, V_{\phi\sigma}, V_{\sigma\phi}, V_{\sigma\sigma}$ are effective interactions (two-body operators) generated by the reduction to the two-particle subspace. From Eq.(14), for the channel wavefunctions, $\psi^{\alpha=\phi,\sigma}_{JM}(\mathbf{r}) \equiv \langle \mathbf{r}|\alpha, JM\rangle$, we obtain

$$\begin{aligned}
\psi^\alpha_{JM}(\mathbf{r}) = &\int d^3\mathbf{r}'\, G^\alpha_0(\mathbf{r}-\mathbf{r}';\sqrt{s})\\
&\times \sum_\beta \int d^3\mathbf{z}\, \tilde{V}_{\alpha\beta}(\mathbf{r}',-\mathbf{z})\, \psi^\beta_{JM}(\mathbf{z}).
\end{aligned}$$

The coupled-channel scattering amplitudes can be defined by

$$\begin{aligned}
f^{\alpha\beta}_J(s) = -\frac{m_\alpha}{i^J}&\int d^3\mathbf{r}' d^3\mathbf{z}\, j_J(k_\alpha r')\, Y^*_{JM}(\hat{\mathbf{r}}')\\
&\times \tilde{V}_{\alpha\beta}(\mathbf{r}',-\mathbf{z})\, \psi^\beta_{JM}(\mathbf{z}), \quad (15)
\end{aligned}$$

where $k_\alpha = \sqrt{s/4 - m^2_\alpha}$ is the magnitude of the relative momentum in the center-of-mass frame of the two particles in channel α. By analogy to the single channel case, the asymptotic wavefunction in channel α is given by

$$\begin{aligned}
\psi^\alpha_{JM}(\mathbf{r}) \to &\frac{\sqrt{s}}{2m_\alpha} Y_{JM}(\hat{\mathbf{r}})\, i^J\\
&\times \left[4\pi\, j_J(k_\alpha r) + i k_\alpha\, h^+_J(k_\alpha r)\textstyle\sum_\beta f^{\alpha\beta}_J(s)\right]. \quad (16)
\end{aligned}$$

The two-channel scattering matrix $f^{\alpha\beta}$ is conventionally parameterizated in terms of two scattering phase-shifts, $\delta^\alpha_J(s)$ ($\alpha = \phi, \sigma$), and an inelasticity, $\eta_J(s)$, representing the fraction of flux exchanged between the two channels,

$$\begin{aligned}
f^{\alpha\alpha}_J(s) &= \frac{4\pi}{k_\alpha}\cdot\frac{\eta_J\, e^{2i\delta^\alpha_J} - 1}{2i};\\
f^{\alpha\beta}_J(s) &= \frac{4\pi}{\sqrt{k_\alpha k_\beta}}\cdot\frac{\sqrt{1-\eta^2_J}\, e^{i(\delta^\alpha_J + \delta^\beta_J)}}{2}.
\end{aligned}$$

Extending the one-channel analysis of the asymptotic states in finite-volume to the two-channel system, one obtains,

$$\begin{aligned}
\psi^{\alpha(L,\mathbf{Q})}_{JM}(\mathbf{r}) \to &\frac{\sqrt{s}}{2m_\alpha}(\text{-}k_\alpha)\, i^J \sum_{J'M'} Y_{J'M'}(\hat{\mathbf{r}})\left[\textstyle\sum_\beta f^{\alpha\beta}_J(s)\right]\\
&\times\left[\delta_{JM,J'M'}\, n_{J'}(k_\alpha r) - \mathcal{M}^{(\mathbf{Q})}_{JM,J'M'}(k_\alpha)\, j_{J'}(k_\alpha r)\right].
\end{aligned} \quad (17)$$

Matching the wavefunctions in finite-volume, Eq. (17), to the wavefunctions in infinite volume, Eq. (16), we can derive the analogue of Eq. (13) for the coupled channel case,

$$\det\begin{bmatrix}
\delta_{JM,J'M'}\,\cot\Delta^\phi_J - \mathcal{M}^{(\mathbf{Q})}_{JM,J'M'}(k_\phi) & \sqrt{\frac{k_\phi}{k_\sigma}}\left[i\,\delta_{JM,J'M'} - \mathcal{M}^{(\mathbf{Q})}_{JM,J'M'}(k_\phi)\right]\frac{\sqrt{1-\eta^2_J}\, e^{i\Delta^\sigma_J}}{2\eta_J\sin\Delta^\phi_J}\\
\sqrt{\frac{k_\sigma}{k_\phi}}\left[i\,\delta_{JM,J'M'} - \mathcal{M}^{(\mathbf{Q})}_{JM,J'M'}(k_\sigma)\right]\frac{\sqrt{1-\eta^2_J}\, e^{i\Delta^\phi_J}}{2\eta_J\sin\Delta^\sigma_J} & \delta_{JM,J'M'}\,\cot\Delta^\sigma_J - \mathcal{M}^{(\mathbf{Q})}_{JM,J'M'}(k_\sigma)
\end{bmatrix} = 0, \quad (18)$$

where $\Delta^\alpha_J(s) \equiv \delta^\alpha_J(s) - \frac{i}{2}\log\eta_J(s)$. One can show that this result is equivalent to Eq.(4.14) in [14]. As in the single-channel case, the subduction of Eq.(18) to irreducible representations of the appropriate little groups can be performed [31].

Eq.(18) is complex and leads to two equations for the three real parameters, $\delta^\phi_J, \delta^\sigma_J, \eta_J$, in each partial wave. Further, under certain conditions, *e.g.* S-wave dominance, Eq.(18) becomes a single real equation in the three unknowns, $(\delta^\phi_0, \delta^\sigma_0, \eta_0)$. Thus additional constraints need to be imposed to obtain a unique solution. For example, in [15] unitarized chiral perturbation was used to constrain amplitude parameters at low energies. In the next section we explore other strategies in the context of an analytical parametrization of the amplitude.

IV. A TOY MODEL OF RESONANT COUPLED-CHANNEL SCATTERING IN FINITE-VOLUME

In order to explore possible strategies for extracting coupled-channel scattering amplitudes from the discrete finite-volume spectra emerging from lattice QCD computations, we consider a simple model of two-channel S-wave scattering. The model is based on resonance-dominated scattering and satisfies the analytical properties required of partial wave amplitudes. With an explicit model for two phase shifts and the inelasticity we can solve Eq. (18) to obtain finite-volume spectra of states as a function of the volume ($V = L^3$) and total momentum of the center-of-mass $\mathbf{P} = 2\pi\mathbf{d}/L$, $\mathbf{d} \in \mathbb{Z}^3$

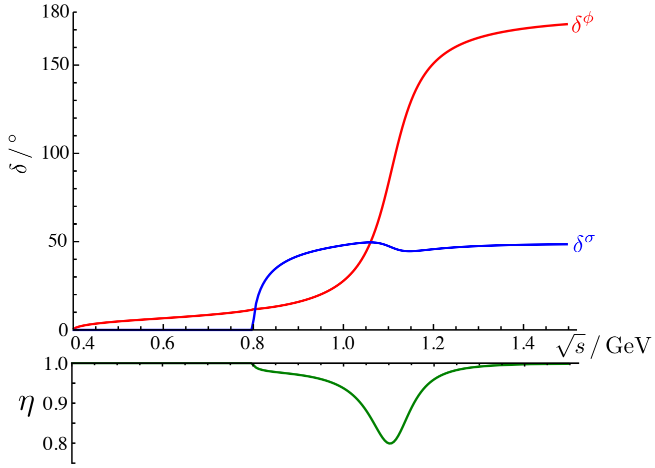

FIG. 1: Phase-shifts and inelasticity for the model defined in the text.

($\mathbf{P} = 2\gamma\mathbf{Q}$). We then use this spectrum as pseudo-data representing a hypothetical lattice QCD simulation and attempt to reproduce the input model.

A. Analytical model of two-channel scattering

We consider a model in which a single S-wave resonance in both channels interferes with a non-resonant background. The two-channel scattering amplitude is parametrized in terms of a K-matrix,

$$K_{\alpha\beta}(s) = \frac{g_\alpha g_\beta}{M^2 - s} + \gamma^{(0)}_{\alpha\beta} + \gamma^{(1)}_{\alpha\beta}\, s + \ldots, \tag{19}$$

which is related to the t-matrix by

$$\left[t^{-1}(s)\right]_{\alpha\beta} = \left[K^{-1}(s)\right]_{\alpha\beta} + \delta_{\alpha\beta}\, I_\alpha(s),$$

and to the scattering amplitude defined in Eq. (15) by $t^{\alpha\beta}_J(s) = \sqrt{s} f^{\alpha\beta}_J(s)/8\pi$ with ($\alpha = \phi, \sigma$). Here $I_\alpha(s)$ is the Chew-Mandelstam form [32], whose imaginary part above threshold, *i.e.* for $s > 4m_\alpha^2$, is given by the phase-space,

$$I_\alpha(s) = I_\alpha(0) - \frac{s}{\pi}\int_{4m_\alpha^2}^{\infty} ds' \sqrt{1 - \frac{4m_\alpha^2}{s'}}\, \frac{1}{(s'-s)s'}.$$

We have opted to subtract the integral once, and it is convenient to choose $I_\alpha(0)$ such that $\mathrm{Re}\, I_\alpha(M^2) = 0$ so that we have an amplitude which for real s near M^2 is close to the Breit-Wigner form with mass M. The t-matrix is an analytical function in the complex s-plane with the discontinuity across the right-hand cut determined by unitarity.

With the following choice of parameters,

$$\begin{aligned} m_\phi = 0.2\,\mathrm{GeV},\ \ m_\sigma = 0.4\,\mathrm{GeV} \\ M = 1.1\,\mathrm{GeV},\ g_\phi = 0.35\,\mathrm{GeV},\ g_\sigma = 0.2\,\mathrm{GeV} \\ \gamma^{(n)}_{\phi\phi} = \gamma^{(n)}_{\phi\sigma} = 0,\ \gamma^{(0)}_{\sigma\sigma} = 0.7,\ \gamma^{(1)}_{\sigma\sigma} = 0.7\,\mathrm{GeV}^{-2},\ \gamma^{(n>1)}_{\sigma\sigma} = 0, \end{aligned}$$

we obtain the phase-shifts and inelasticity shown in Fig. 1. The parameters have been chosen in such a way that there is a narrow resonance near $s = (1.1\,\mathrm{GeV})^2$. It is usual to analyse scattering in terms of the most relevant singularities of the t-matrix on the nearby unphysical sheets. Poles on unphysical sheets are often identified with hadron resonances. In this case the four sheets ($\mathsf{sheet\,I}$ is the physical sheet) can be defined by

$$\left[t^{-1}_{\mathsf{sheet}}(s)\right]_{\alpha\beta} = \begin{cases} \left[t^{-1}_{\mathsf{I}}(s)\right]_{\alpha\beta} & \mathsf{sheet\ I} \\ \left[t^{-1}_{\mathsf{I}}(s)\right]_{\alpha\beta} + 2i\sqrt{1-\frac{4m_\phi^2}{s}}\,\delta_{\alpha\phi} & \mathsf{sheet\ II} \\ \left[t^{-1}_{\mathsf{I}}(s)\right]_{\alpha\beta} + 2i\sqrt{1-\frac{4m_\alpha^2}{s}}\,\delta_{\alpha\beta} & \mathsf{sheet\ III} \\ \left[t^{-1}_{\mathsf{I}}(s)\right]_{\alpha\beta} + 2i\sqrt{1-\frac{4m_\sigma^2}{s}}\,\delta_{\alpha\sigma} & \mathsf{sheet\ IV} \end{cases}.$$

The model amplitude has a single pole on each of sheets II and III, with the t-matrix in the neighbourhood of the pole at s_0 behaving like,

$$\left[t_{\mathsf{sheet}}(s \to s_0)\right]_{\alpha\beta} \to \frac{c_\alpha c_\beta}{s_0 - s},$$

with

$$\begin{aligned} &\sqrt{s_0} = \left(1.1072 - \tfrac{i}{2}0.0888\right)\mathrm{GeV} \\ &c_\phi = \left(0.3511\,\mathrm{GeV}\right)e^{-i0.0018\pi},\ c_\sigma = \left(0.1339\,\mathrm{GeV}\right)e^{-i0.238\pi} \end{aligned}$$

on $\mathsf{sheet\,II}$ and

$$\begin{aligned} &\sqrt{s_0} = \left(1.1083 - \tfrac{i}{2}0.1096\right)\mathrm{GeV} \\ &c_\phi = \left(0.3499\,\mathrm{GeV}\right)e^{+i0.0009\pi},\ c_\sigma = \left(0.1396\,\mathrm{GeV}\right)e^{+i0.249\pi} \end{aligned}$$

on $\mathsf{sheet\,III}$. Our aim is to use the finite-volume spectrum determined on a set of volumes and total momenta, $\mathbf{P}$, to reproduce the pole positions of this scattering amplitude.

B. Finite-volume spectrum

The finite-volume spectrum corresponding to the model defined in the previous section can be obtained by solving Eq. (13) for energies $E = \sqrt{s} < 2m_\sigma$ and Eq. (18) for energies above $2m_\sigma$. Restriction to S-wave scattering reduces Eq. (18) to,

$$\begin{aligned} 0 &= \Omega(\delta^\phi(E), \delta^\sigma(E), \eta(E); L, \mathbf{d}; E) \\ &= \eta\left[\mathcal{M}_\phi - \mathcal{M}_\sigma\right]\sin\left(\delta^\phi - \delta^\sigma\right) \\ &\quad + \left[\mathcal{M}_\phi + \mathcal{M}_\sigma\right]\sin\left(\delta^\phi + \delta^\sigma\right) \\ &\quad - \eta\left[1 + \mathcal{M}_\phi\,\mathcal{M}_\sigma\right]\cos\left(\delta^\phi - \delta^\sigma\right) \\ &\quad - \left[1 - \mathcal{M}_\phi\,\mathcal{M}_\sigma\right]\cos\left(\delta^\phi + \delta^\sigma\right), \end{aligned} \tag{20}$$

where $\mathcal{M}_\phi \equiv \mathcal{M}^{(\mathbf{Q})}_{J=0\,M=0, J'=0\,M'=0}(k_\phi)$ with a similar expression for $\mathcal{M}_\sigma$. $\mathbf{Q}$ is a function of $\mathbf{d}$, L, E as discussed in Sec. II B. In Fig.2 we show the finite-volume spectrum obtained by solving Eq. (13) and (18) as a function of the volume in a region $L = 16 - 24\,\mathrm{GeV}^{-1}$ (or $L = 3.2 - 4.7$ fm).

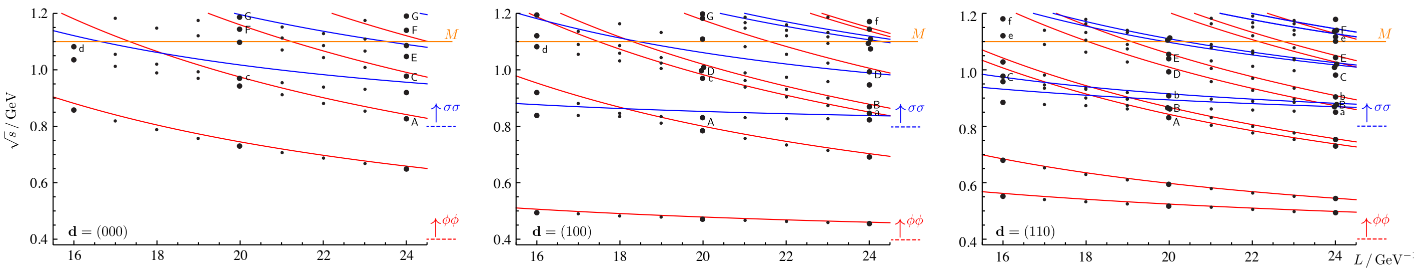

FIG. 2: Finite-volume spectra for the K-matrix model described in Sec. IV A. Black dots indicate the spectrum obtained by solving Eqs. (13), (18). Red and blue curves represent the energy of a non-interacting pair of mesons ($\alpha = \phi, \sigma$) $\left[\left(\sqrt{m_\alpha^2 + \mathbf{k}_1^2} + \sqrt{m_\alpha^2 + \mathbf{k}_2^2}\right)^2 - \mathbf{P}^2\right]^{1/2}$, $\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{P}$ and $\mathbf{k} = \frac{2\pi}{L}\mathbf{n}, \mathbf{n} \in \mathbb{Z}^3$.

C. "Pointwise" estimation of scattering from finite-volume spectrum

One approach to determining the phase-shifts and inelasticities at discrete values of energy is to locate multiple energy levels (in different volumes and/or different $\mathbf{d}$) that appear at approximately the same energy. As an example consider the three levels labeled A in Fig. 2 which all lie within 2 MeV of $\sqrt{s} = 830\,\mathrm{MeV}$. For the three levels we can build three independent copies of Eq. (18) which each feature approximately the same values of $\delta^\phi(s), \delta^\sigma(s), \eta(s)$, which can be determined by solving the set of simultaneous equations. Since the energies are not *exactly* degenerate, there need not be an exact solution to the equations and hence we seek to find the solution which minimizes

$$\sum_{E(L,\mathbf{d})} \left|\Omega(\delta^\phi, \delta^\sigma, \eta; L, \mathbf{d}; E)\right|^2,$$

with Ω defined in Eq. (20) and where the sum is over the three energy levels. For the levels A, the obtained solution, as shown in Fig. 3, is within 3% of the exact value of $\delta^\phi(s_A), \delta^\sigma(s_A), \eta(s_A)$.

Within the energy region considered, $E = 0.8 - 1.2\,\mathrm{GeV}$, considering only three volumes, $L = 16, 20, 24\,\mathrm{GeV}^{-1}$, and three sets of center-of-mass momentum, $\mathbf{d} = (000), (100), (110)$, we can isolate a number of such sets. These sets of three near-degenerate energy levels are labelled $\mathsf{A} - \mathsf{G}$ in Fig. 2. In Fig. 3 the labels are shown on the plot of δ^ϕ with the corresponding solutions for δ^σ and η marked by solid dots.

With these points alone, in Fig. 3 we see strong hints of a signal for resonant behavior in the δ^ϕ phase shift. While obviously resonably successful, this approach does not make optimal use of the finite-volume spectral information, by failing to use any energy level which does not have two near-degenerate partners. To use more of the discrete levels we might consider building a system of *two* instances of Eq. (18) with one parameter from the set $\delta^\phi, \delta^\sigma, \eta$, estimated using interpolation between already determined values. For example consider the two levels near 1.117 GeV labeled d in Fig. 2. Linear interpolation between the energies of the E and F points in Fig. 3 gives $\delta^\phi(1.117\,\mathrm{GeV}) = 102.3°$. Using this value and minimizing with respect to δ^σ, η at the energy corresponding to point d we obtain $\delta^\sigma = 46.2°, \eta = 0.800$. A spline interpolation using all the points $\mathsf{A} - \mathsf{G}$ yields $\delta^\phi(1.117\,\mathrm{GeV}) = 102.2°$ which results in $\delta^\sigma = 46.3°, \eta = 0.799$ at the point d. In Fig. 3 we show the results for sets of two degenerate levels labeled $\mathsf{a} - \mathsf{f}$ from Fig. 2. In each case the errorbars represent limiting values obtained using two methods of interpolation. Even though in some cases there is a considerable sensitivity to the interpolation method, overall the points are in reasonable agreement with the model input (solid light-colored curves).

D. Parameterized estimation of scattering from finite-volume spectrum

The previously discussed "pointwise" strategy, while having the advantage of being largely model-independent, is reliant upon there being multiple energy levels which, through accident or design, are close to degenerate. Since it would be unusual to engineer lattice volumes purely for this purpose, it is appropriate to consider alternative methods of analysis. One such approach that makes full use of all determined levels involves parameterising the scattering amplitude and performing a minimisation to get the best description of the determined finite-volume spectrum by varying the parameters. In the current toy-model, even limited "pointwise" analysis would suggest that the phase δ^ϕ is rapidly rising and would indicate that a resonance could be present. By including a pole (as well as polynomial behaviour) in a K-matrix we are likely to get rapid convergence to a solution with a pole in the t-matrix.

We will take this opportunity to make the toy model a slightly more realistic simulation of an actual lattice QCD calculation by introducing statistical uncertainty on the energy level values. In recent work [22], [6], the Hadron Spectrum Collaboration has obtained sta-

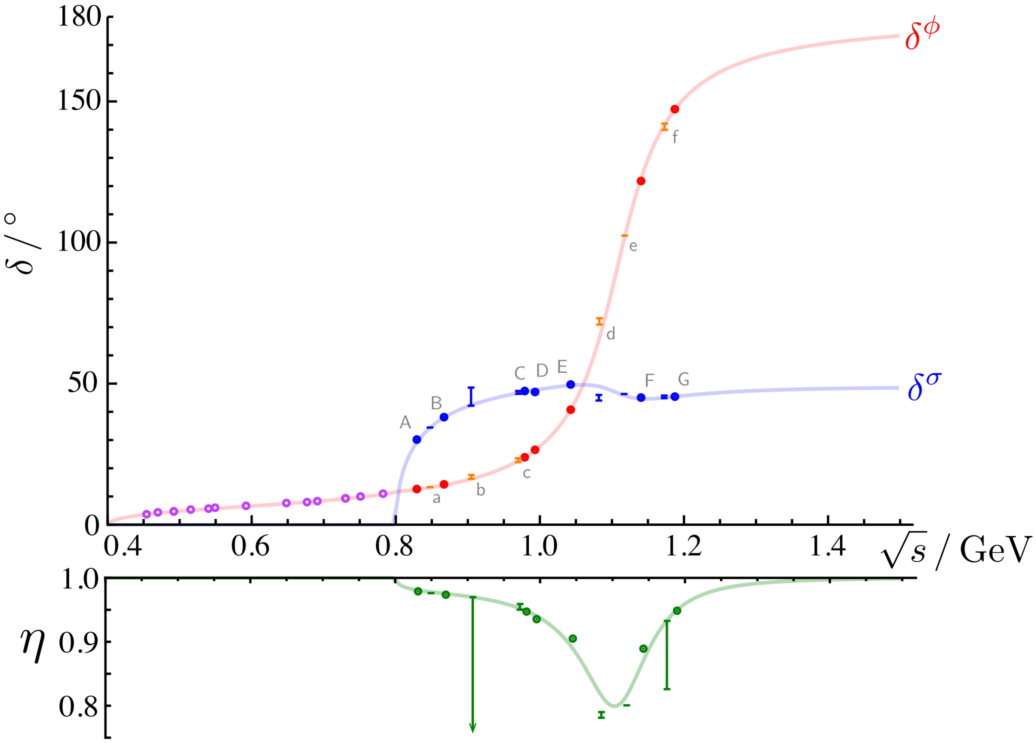

FIG. 3: "Pointwise" determination of the phase-shifts and inelasticity. Energies A − G determined from constrained three-level analysis, energies a − f by interpolation in δ^ϕ from two-level analysis. The light-colored curves show the exact input model.

tistical errors on excited levels as small as 0.3% and we will assume that this remains practical. For each energy level below 1.2 GeV on volumes $L = 16, 20\,\mathrm{GeV}^{-1}$ with $\mathbf{d} = (000), (100), (110)$, we randomly generated an ensemble by drawing from a distribution whose mean is the exact value given in Fig. 2 and whose variance is chosen such that the ensemble has variance on the mean of 0.3% of the mean value. The resulting spectrum is shown in Fig. 4.

Parametrizing according to the form given in Eq. (19), we can minimise a function,

$$\chi^2(\{a_i\}) = \sum_{E_\mathfrak{n}(L,\mathbf{d})} \frac{\left[E_\mathfrak{n}(L,\mathbf{d}) - E^{\mathrm{det}}_\mathfrak{n}(L,\mathbf{d};\{a_i\})\right]^2}{\sigma(E_\mathfrak{n}(L,\mathbf{d}))^2},$$

(where E^{det} are the solutions of Eqs. (13) and (18)), by varying the parameters of the K-matrix, $\{a_i\} = \{M, g_\phi, g_\sigma, \gamma^{(n)} \ldots\}$. In practical lattice QCD calculations, the χ^2 can be trivially adjusted to deal with correlated data by replacing the diagonal variance by the inverse of the data covariance matrix.

In Fig.5 we show the parameterized phase-shifts and inelasticity obtained using three models:

- A: "exact model", which uses a 1st order polynomial in s to describe the non-pole contribution to the K-matrix with $\gamma^{(0,1)}_{\phi\phi} = \gamma^{(0,1)}_{\phi\sigma} \equiv 0$ [5 parameters]

- B: "relaxed model", with 1st order polynomial in all channels *i.e.* all $\gamma^{(0,1)}$ free [9 parameters]

- C: "tight model", with 0th order of polynomials in all channels *i.e.* $\gamma^{(1)} = 0$ [6 parameters].

As one would expect, within statistical uncertainty, parameterization A reproduces the input model. Parameterisation B, which is more flexible, also reproduces the input quite well over the energy region where data is given, but begins to deviate from the original K-matrix in the energy range outside of the fit region. Parameterization C does not have sufficient flexibility to describe the complete energy dependence, and it fails to describe δ^σ at high energies, away from the energy region where the pole dominates.

Our principal interest lies in identifying resonances as poles in the complex-s plane - analytically continuing the fitted model amplitudes we find that all three have single poles on sheets II and III whose locations are in a rather good agreement with the input pole position (see Fig. 6). The residues at the pole agree similarly.

In summary, the "pointwise" strategy may provide a less model-dependent approach for extracting phase shifts and inelasticities, however, this method is limited by the number of points for which accidental degeneracies appear. Parameterizing the scattering amplitude allow us to make use of all measured energy levels, how-

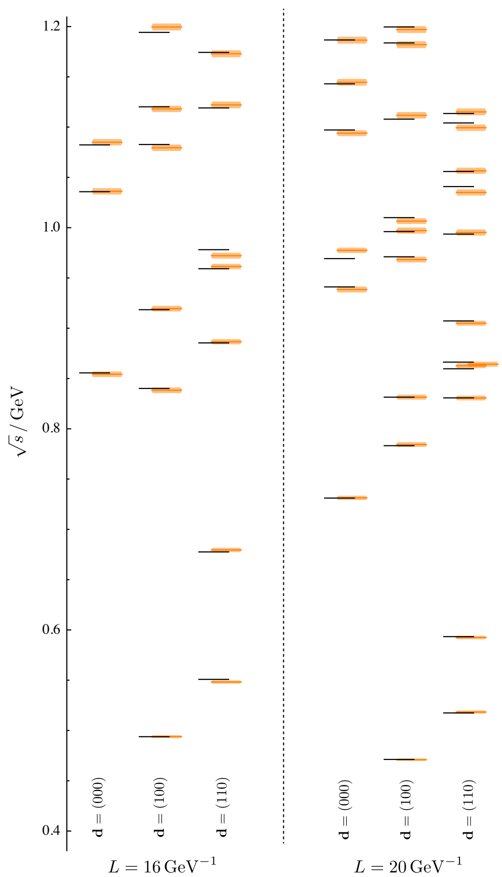

FIG. 4: Orange rectangles: finite-volume spectra with 0.3% noise. Black lines: exact finite-volume spectrum given in Fig.2.

ever we need to find suitable parameterizations. One strategy is to explore the "pointwise" approach to find a crude guide to the energy dependence and then build parameterizations which are able to reproduce the obtained form. The parameterizations, which should respect certain constraints applicable to scattering amplitudes, can be made progressively more sophisticated in an effort to reduce the overall χ^2 - in this sense the approach is not dissimilar to what is done with real experimental data.

V. THREE-PARTICLE SCATTERING ON A TORUS WITHIN AN ISOBAR APPROXIMATION

In the previous section we considered only two-particle Fock states in the inelastic region, however in QCD, because of the low mass of pions, three-particle states become important at relatively low energies. Methods for extracting three-particle amplitudes from lattice simulations are thus also needed. In general, the scattering of a multiple-particle system is quite complicated, however, in some cases the quasi-two body approximation has proven to be quite successful [33, 34]. A recent consideration of the three-particle system on a torus in the framework of Faddeev equations is presented in [35].

In the presence of two-body resonances, the three-particle system can be approximately described in terms of isobars [26, 27, 36, 37], for example, the decay process of $K_1(1400)$ to the $K\pi\pi$ final state can be quite well approximated by $K^*(892)\pi$ in S-wave, with the K^* isobar decaying to $K\pi$ in a P-wave.

In this section, we will generalize the previously introduced methods to the three-particle system in the isobar approximation. For simplicity we consider three scalars with equal masses, m. Under the assumption of strong pair-wise interactions between two particles, the Hamiltonian of the three-particle system takes the form

$$H = \sum_{k=1,2,3} \sqrt{\mathbf{p}_k^2 + m^2} + \sum_{k=1,2,3}^{i\neq j\neq k} \tilde{V}(\mathbf{x}_i - \mathbf{x}_j)$$

where $(\mathbf{p}_k, \mathbf{x}_k)$ are the momentum and coordinate of the k-th particle. In the center-of-mass frame, the wavefunction of the three-particle system has the following form [34]

$$\psi_{JM}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = \sum_{k=1,2,3}^{i\neq j\neq k} \phi^{(ij)}_{JM}(\mathbf{r}_{ij}, \mathbf{r}_k),$$

where $\mathbf{r}_{ij} = \mathbf{x}_i - \mathbf{x}_j$ is the relative position between two particles forming the (ij) isobar and $\mathbf{r}_k = \frac{1}{2}(\mathbf{x}_i + \mathbf{x}_j) - \mathbf{x}_k$ is the relative position of the spectator particle and the isobar. The solution of the Schrödinger equation $\hat{H}\psi_{JM} = E\psi_{JM}$ is given by

$$\phi^{(ij)}_{JM}(\mathbf{r}_{ij}, \mathbf{r}_k) = \int d^3\mathbf{r}'_{ij}\, d^3\mathbf{r}'_k\, G_0(\mathbf{r}_{ij} - \mathbf{r}'_{ij}, \mathbf{r}_k - \mathbf{r}'_k; E) \times \tilde{V}_{ij}(\mathbf{r}'_{ij})\, \psi_{JM}(\mathbf{x}'_1, \mathbf{x}'_2, \mathbf{x}'_3),$$

with G_0 being the relativistic three-body Green's function,

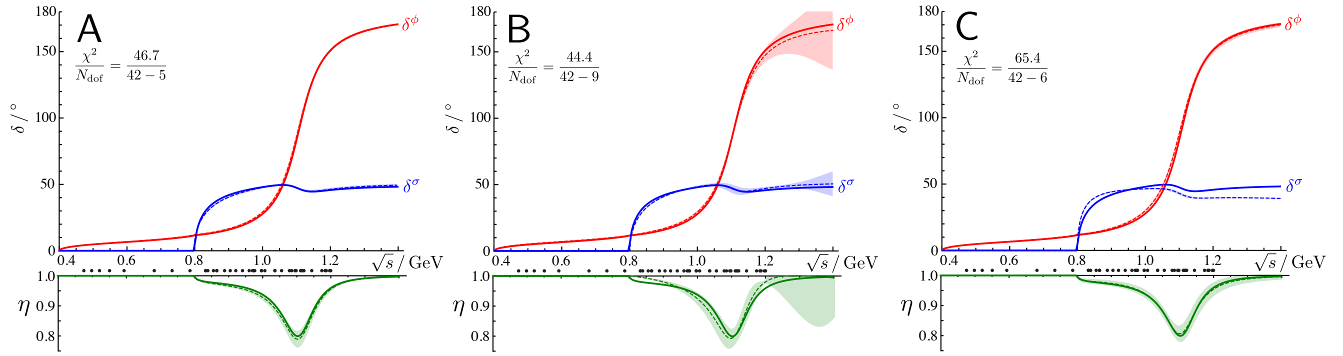

FIG. 5: Best-fit phase-shifts and inelasticity for the parameterizations A − C as described in the text shown by dashed curves and error bands. Exact input forms shown by solid lines. Black dots indicate the positions of the energy levels used in the χ^2 minimization.

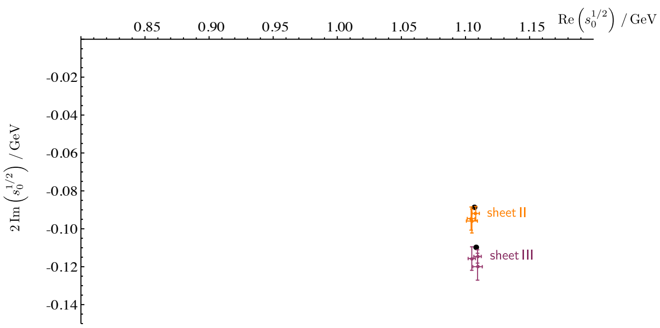

FIG. 6: Poles of the t-matrix on sheets II, III determined from parameterizations A − C as described in the text. Black dots show the exact poles of the input model.

$$G_0(\mathbf{r}_{ij}, \mathbf{r}_k; E) = \int \frac{d^3\mathbf{q}_{ij}}{(2\pi)^3} \frac{d^3\mathbf{k}_k}{(2\pi)^3} \frac{e^{i\mathbf{q}_{ij}\cdot\mathbf{r}_{ij} + i\mathbf{k}_k\cdot\mathbf{r}_k}}{E - \sqrt{m^2 + \mathbf{k}_k^2} - \sqrt{m^2 + \left(\frac{1}{2}\mathbf{k}_k + \mathbf{q}_{ij}\right)^2} - \sqrt{m^2 + \left(\frac{1}{2}\mathbf{k}_k - \mathbf{q}_{ij}\right)^2}}.$$

In the isobar approximation, interactions within the three-particle system can be described by two types of process: interactions between the isobar pair and the spectator, $(ij) + k \leftrightarrow (ij) + k$, with all possible arrangements, and interactions between particles within the isobar, $i \leftrightarrow j$. This enables us to represent the full three-body Green's function by a product of two independent two-body Green's functions

$$G_0(\mathbf{r}_{ij}, \mathbf{r}_k; E) \simeq \frac{i}{2\pi} \int_{-\infty}^{\infty} dE_{ij}\, G_0^{(ij)+k}(\mathbf{r}_k; E)\, G_0^{i+j}(\mathbf{r}_{ij}; E_{ij}),$$

where

$$G_0^{(ij)+k}(\mathbf{r}_k; E) = \int \frac{d^3\mathbf{k}_k}{(2\pi)^3} \frac{e^{i\mathbf{k}_k\cdot\mathbf{r}_k}}{E - \sqrt{m^2 + \mathbf{k}_k^2} - \sqrt{E_{ij}^2 + \mathbf{k}_k^2}}$$

is the free Green's function for propagation of the system, of total energy E, made of the isobar pair (ij) (with invariant mass E_{ij}) plus the spectator particle, and where

$$G_0^{i+j}(\mathbf{r}_{ij}; E_{ij}) = \int \frac{d^3\mathbf{q}_{ij}}{(2\pi)^3} \frac{e^{i\mathbf{q}_{ij}\cdot\mathbf{r}_{ij}}}{E_{ij} - 2\sqrt{m^2 + \mathbf{q}_{ij}^2}},$$

is the free Green's function describing the propagation of particles, (i, j), inside the isobar.

The Green's functions, excluding any pieces which decay exponentially with distance, are explicitly given by

$$G_0(\mathbf{r}_{ij}, \mathbf{r}_k; E) \to -\frac{1}{2\pi i} \int_{2m}^{E-m} dE_{ij}\, \frac{E_{ij}}{E} \frac{1}{(4\pi)^2} \times \sqrt{(k_{E_{ij}}^2 + m^2)(k_{E_{ij}}^2 + E_{ij}^2)}\, \frac{e^{iq_{E_{ij}} r_{ij}}}{r_{ij}} \frac{e^{ik_{E_{ij}} r_k}}{r_k}, \tag{21}$$

with

$$q_{E_{ij}} = \tfrac{1}{2}\sqrt{E_{ij}^2 - 4m^2},$$
$$k_{E_{ij}} = \frac{\sqrt{[E^2-(m-E_{ij})^2]\,[E^2-(m+E_{ij})^2]}}{2E}.$$

In Eq.(21), $\int_{-\infty}^{\infty} dE_{ij}$ has been replaced by $\int_{2m}^{E-m} dE_{ij}$, because the three-body Green's function has oscillatory behavior for E_{ij} only inside the physical region. The asymptotic behavior of the three-particle wavefunction is given by

$$\begin{aligned}&\psi_{JM}(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)\\ &\quad\to -\frac{1}{2\pi i}\sum_{k=1,2,3}\int_{2m}^{E-m} dE_{ij}\sum_{\substack{S_{ij}M_{S_{ij}}\\ L_k M_{L_k}}}\\ &\quad\times (iq_{E_{ij}})\, h^+_{S_{ij}}(q_{E_{ij}} r_{ij})\, i^{S_{ij}}\, Y_{S_{ij}M_{S_{ij}}}(\hat{\mathbf{r}}_{ij})\\ &\quad\times (ik_E)\, h^+_{L_k}(k_{E_{ij}} r_k)\, i^{L_k}\, Y_{L_k M_{L_k}}(\hat{\mathbf{r}}_k)\\ &\quad\times f^{(ij)}_{JM;S_{ij}M_{S_{ij}};L_k M_{L_k}}(q_{E_{ij}}, k_{E_{ij}}),\end{aligned}$$

where the three-body scattering amplitudes are defined by

$$\begin{aligned}&f^{(ij)}_{JM;S_{ij}M_{S_{ij}};L_k M_{L_k}}(q_{E_{ij}}, k_{E_{ij}})\\ &\quad= \frac{E_{ij}}{E}\sqrt{(k^2_{E_{ij}}+m^2)(k^2_{E_{ij}}+E^2_{ij})}\int d^3\mathbf{r}'_{ij}\, d^3\mathbf{r}'_k\\ &\quad\times i^{-S_{ij}}\, j_{S_{ij}}(q_{E_{ij}} r'_{ij})\, Y^*_{S_{ij}M_{S_{ij}}}(\hat{\mathbf{r}}'_{ij})\\ &\quad\times i^{-L_k}\, j_{L_k}(k_{E_{ij}} r'_k)\, Y^*_{L_k M_{L_k}}(\hat{\mathbf{r}}'_k)\\ &\quad\times \tilde{V}_{ij}(\mathbf{r}'_{ij})\, \psi_{JM}(\mathbf{x}'_1,\mathbf{x}'_2,\mathbf{x}'_3). \qquad (22)\end{aligned}$$

The total angular momentum of the three-particle system is J, made up of $(S_{ij}, M_{S_{ij}})$, the spin and its z-axis projection of the isobar pair (ij), and (L_k, M_{L_k}), the relative orbital angular momentum and projection between k-th particle and isobar pair (ij).

The partial wave amplitude can be parametrized by

$$\begin{aligned}&f^{(ij)}_{JM;S_{ij}M_{S_{ij}};L_k M_{L_k}}(q_{E_{ij}}, k_{E_{ij}})\\ &\quad= \langle S_{ij}M_{S_{ij}}; L_k M_{L_k}|JM\rangle\, f_{S_{ij}}(q_{E_{ij}})\, f_{S_{ij}L_k J}(k_{E_{ij}}), \qquad (23)\end{aligned}$$

where

$$f_{S_{ij}}(q_{E_{ij}}) = \frac{4\pi}{q_{E_{ij}}} e^{i\delta_{S_{ij}}}\sin\delta_{S_{ij}},$$

is the partial wave scattering amplitude of two spinless particles inside the isobar pair (ij) and

$$f_{S_{ij}L_k J}(k_{E_{ij}}) = \frac{4\pi}{k_{E_{ij}}} e^{i\delta_{S_{ij}L_k J}}\sin\delta_{S_{ij}L_k J}$$

is the partial wave scattering amplitude of the isobar pair (ij) and the spectator particle.

The final expression for the three-particle wave function, including the homogeneous term, reads

$$\begin{aligned}\psi_{JM}(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3) \to \frac{i}{2\pi}\sum_{k=1,2,3}\sum_{\substack{S_{ij}M_{S_{ij}}\\ L_k M_{L_k}}} &\langle S_{ij}M_{S_{ij}}; L_k M_{L_k}|JM\rangle\, Y_{S_{ij}M_{S_{ij}}}(\hat{\mathbf{r}}_{ij})\, Y_{L_k M_{L_k}}(\hat{\mathbf{r}}_k)\\ &\times \int_{2m}^{E-m} dE_{ij}\; i^{S_{ij}}\left[(4\pi)\, j_{S_{ij}}(q_{E_{ij}} r_{ij}) + i\, q_{E_{ij}}\, h^+_{S_{ij}}(q_{E_{ij}} r_{ij})\, f_{S_{ij}}(q_{E_{ij}})\right]\\ &\times i^{L_k}\left[(4\pi)\, j_{L_k}(k_{E_{ij}} r_k) + i\, k_{E_{ij}}\, h^+_{L_k}(k_{E_{ij}} r_k)\, f_{S_{ij}L_k J}(k_{E_{ij}})\right].\end{aligned}$$

When considering three particles in a cubic finite-volume we may choose the following boundary condition on the wavefunction

$$\psi^{(L)}_{JM}(\mathbf{r}_{ij} + \mathbf{n}_{ij}L, \mathbf{r}_k + \mathbf{n}_k L) = e^{i\mathbf{Q}\cdot\mathbf{n}_k L}\, \psi^{(L)}_{JM}(\mathbf{r}_{ij}, \mathbf{r}_k),$$

where $k = 1,2,3$ and $\mathbf{Q}$ is the Bloch wave vector for the three-particle system. Boosting the three-particle system from the center-of-mass frame to a lab frame with the center-of-mass of isobar pair (ij) fixed at the origin, $\mathbf{x}_i + \mathbf{x}_j = \mathbf{0}$, the wavefunction of the three-particle system at the lab frame can be written as the product of a plane-wave, $e^{i\mathbf{P}\cdot(\mathbf{x}_1+\mathbf{x}_2+\mathbf{x}_3)/3}$, and a piece depending only on relative coordinates, $\mathbf{r}_{ij} = \mathbf{x}_i - \mathbf{x}_j$ and $\mathbf{r}_k = -\mathbf{x}_k$. As in the case of two-particle scattering [9], requiring periodicity of the lab frame wavefunction with respect to $\mathbf{r}_{ij}$ and $\mathbf{r}_k$, we find the connection of the Bloch wave vector $\mathbf{Q}$ to the total momentum of the three-particle system, $\mathbf{P} = 3\gamma\mathbf{Q}$. Using the periodicity of the potential $\tilde{V}_{ij}(\mathbf{r}'_{ij} + \mathbf{n}_{ij}L) = \tilde{V}_{ij}(\mathbf{r}'_{ij})$, the three-particle Lippmann-Schwinger equation on a torus can

be written

$$\psi^{(L,\mathbf{Q})}_{JM}(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)=\sum_{k=1,2,3}\int_{L^3} d^3\mathbf{r}'_{ij}\int_{L^3} d^3\mathbf{r}'_k\, G_{\mathbf{Q}}(\mathbf{r}_{ij}-\mathbf{r}'_{ij},\mathbf{r}_k-\mathbf{r}'_k;E)\,\tilde{V}_{ij}(\mathbf{r}'_{ij})\,\psi^{(L,\mathbf{Q})}_{JM}(\mathbf{x}'_1,\mathbf{x}'_2,\mathbf{x}'_3),$$

where the periodic three-body Green's function is given by

$$G_{\mathbf{Q}}(\mathbf{r}_{ij},\mathbf{r}_k;E)=\sum_{\mathbf{n}_{ij},\mathbf{n}_k\in\mathbb{Z}^3} G_0(\mathbf{r}_{ij}-\mathbf{n}_{ij}L,\mathbf{r}_k-\mathbf{n}_kL;E)\,e^{i\mathbf{Q}\cdot\mathbf{n}_kL},$$

or asymptotically

$$G_{\mathbf{Q}}(\mathbf{r}_{ij},\mathbf{r}_k;E)\to-\frac{1}{2\pi i}\int_{2m}^{E-m}dE_{ij}\frac{E_{ij}}{E}\sqrt{(k^2_{E_{ij}}+m^2)(k^2_{E_{ij}}+E^2_{ij})}\,\frac{1}{L^3}\sum_{\mathbf{q}_{ij}\in\mathbf{P_0}}\frac{e^{i\mathbf{q}_{ij}\cdot\mathbf{r}_{ij}}}{q^2_{E_{ij}}-\mathbf{q}^2_{ij}}\,\frac{1}{L^3}\sum_{\mathbf{k}_k\in\mathbf{P_Q}}\frac{e^{i\mathbf{k}_k\cdot\mathbf{r}_k}}{k^2_{E_{ij}}-\mathbf{k}^2_k}.$$

Next, we use the expansion of the Green's function in Eq.(B2) and the definition of the scattering amplitude in Eq.(22) and (23), to obtain

$$\begin{aligned}\psi^{(L,\mathbf{Q})}_{JM}(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)\to\frac{i}{2\pi}&\sum_{k=1,2,3}\sum_{\substack{S_{ij}M_{S_{ij}}\\L_kM_{L_k}}}\sum_{\substack{S'_{ij}M'_{S_{ij}}\\L'_kM'_{L_k}}}\langle S_{ij}M_{S_{ij}};L_kM_{L_k}|JM\rangle\,Y_{S'_{ij}M'_{S_{ij}}}(\hat{\mathbf{r}}_{ij})\,Y_{L'_kM'_{L_k}}(\hat{\mathbf{r}}_k)\\&\times\int_{2m}^{E-m}dE_{ij}\,i^{S_{ij}}\,q_{E_{ij}}\,f_{S_{ij}}(q_{E_{ij}})\left[\delta_{S_{ij}M_{S_{ij}},S'_{ij}M'_{S_{ij}}}\,n_{S'_{ij}}(q_{E_{ij}}r_{ij})-\mathcal{M}^{(\mathbf{0})}_{S_{ij}M_{S_{ij}},S'_{ij}M'_{S_{ij}}}(q_{E_{ij}})\,j_{S'_{ij}}(q_{E_{ij}}r_{ij})\right]\\&\qquad\times i^{L_k}\,k_{E_{ij}}\,f_{S_{ij}L_kJ}(k_{E_{ij}})\left[\delta_{L_kM_{L_k},L'_kM'_{L_k}}\,n_{L'_k}(k_{E_{ij}}r_k)-\mathcal{M}^{(\mathbf{Q})}_{L_kM_{L_k},L'_kM'_{L_k}}(k_{E_{ij}})\,j_{L'_k}(k_{E_{ij}}r_k)\right].\end{aligned}$$

Matching a general wavefunction of form $\sum_{JM}c_{JM}\,\psi_{JM}(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)$ with $\sum_{JM}c_{JM}\,\psi^{(L,\mathbf{Q})}_{JM}(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)$, and projecting out the partial waves, neglecting rearrangement effects from crossed channels as appropriate in an isobar approximation, we get a set of equations which have general form $\int_{2m}^{E-m}dE_{ij}\;F(E_{ij},r_{ij},r_k)=0$. Since the variables (r_{ij},r_k) can be chosen arbitrarily, $F(E_{ij},r_{ij},r_k)=0$ must be satisfied for each E_{ij}. From this we obtain three determinant conditions, the first is

$$\det\left[\delta_{S_{ij}M_{S_{ij}},S'_{ij}M'_{S_{ij}}}\,\cot\delta_{S_{ij}}(q_{E_{ij}})-\mathcal{M}^{(\mathbf{0})}_{S_{ij}M_{S_{ij}},S'_{ij}M'_{S_{ij}}}(q_{E_{ij}})\right]=0,\tag{24}$$

which is Lus̆cher's formula for scattering between i-th and j-th particles inside the isobar pair (ij). It provides the constraint on the phase shifts $\delta_{S_{ij}}$ as a function of invariant mass of the isobar pair (ij), E_{ij}. The second condition,

$$\begin{aligned}\det\Bigg[&\delta_{JM,J'M'}\,\delta_{L_k,L'_k}\,\cot\delta_{S_{ij}L_kJ}(k_{E_{ij}})\\&-\sum_{M_{S_{ij}}M_{L_k}M'_{L_k}}\langle S_{ij}M_{S_{ij}};L'_kM'_{L_k}|J'M'\rangle\,\langle S_{ij}M_{S_{ij}};L_kM_{L_k}|JM\rangle\,\mathcal{M}^{(\mathbf{Q})}_{L_kM_{L_k},L'_kM'_{L_k}}(k_{E_{ij}})\Bigg]=0,\end{aligned}\tag{25}$$

is a generalized Lus̆cher's formula in moving frames for scattering between the spectator, k-th particle, and the isobar (ij) with the specific spin S_{ij} and mass E_{ij}. Thus, Eq. (25) gives the constraint on the phase shifts $\delta_{S_{ij}L_kJ}$ as function of the total energy, E, for each individual partial wave of isobar pair (ij), S_{ij}.

The final condition,

$$\begin{aligned}\det\Bigg[&\delta_{JM,J'M'}\,\delta_{S_{ij},S'_{ij}}\,\delta_{L_k,L'_k}\,\cot\delta_{S_{ij}}(q_{E_{ij}})\,\cot\delta_{S_{ij}L_kJ}(k_{E_{ij}})\\&-\sum_{\substack{M_{S_{ij}}M'_{S_{ij}}\\M_{L_k}M'_{L_k}}}\langle S'_{ij}M'_{S_{ij}};L'_kM'_{L_k}|J'M'\rangle\,\langle S_{ij}M_{S_{ij}};L_kM_{L_k}|JM\rangle\,\mathcal{M}^{(\mathbf{0})}_{S_{ij}M_{S_{ij}},S'_{ij}M'_{S_{ij}}}(q_{E_{ij}})\,\mathcal{M}^{(\mathbf{Q})}_{L_kM_{L_k},L'_kM'_{L_k}}(k_{E_{ij}})\Bigg]=0,\end{aligned}\tag{26}$$

leads to an additional constraint on both $\delta_{S_{ij}}$ and $\delta_{S_{ij}L_kJ}$ for the scattering between the k-th particle and all the allowed partial waves of the isobar (ij).

In the case that only a single partial wave S_{ij} of the isobar pair is dominant, Eq. (26) becomes redundant and

the three conditions reduce to two,

$$\cot \delta_{S_{ij}}(q_{E_{ij}}) = \mathcal{M}^{(\mathbf{0})}_{S_{ij}M_{S_{ij}},S'_{ij}M'_{S_{ij}}}(q_{E_{ij}}),$$

and Eq. (25). Similar to the discussion in Section II and III, Eq. (24), (25) and (26) have to be subduced according to irreducible representations of the appropriate little groups [31].

From Eq. (24), (25) and (26), we find that even in relatively simple cases, *e.g.* a single isobar dominating a single relevant partial wave, extracting the phase-shifts and determining the invariant mass E_{ij} from the measured total three-particle energy E is a rather difficult task. For additional information, we can first perform computations of two-particle correlators with the quantum numbers of the isobar channel to obtain information on E_{ij}. However, in the three-body calculation, there may be multiple E_{ij} for each individual E allowed by kinematics ($2m < E_{ij} < E - m$), thus, finding the correspondence between E_{ij} and E may requires some assumptions and model input.

In recent works [4, 5], determining the spin of the excited states by considering the overlap of carefully constructed operators with the particular state, $\langle n|\mathcal{O}|0\rangle$, has been proven to be successful in certain cases. We may use a similar idea to identify the E_{ij} and E relation in a three-particle system, by considering the overlap of operators with the state having the particular quantum numbers (S_{ij}, L_k, J) and invariant mass of the isobar pair E_{ij}. For instance, working in center-of-mass frame, the three-particle operator may be constructed in such way that an isobar pair (ij) has definite relative momentum, $\frac{1}{2}|\mathbf{p}_i - \mathbf{p}_j| = \frac{2\pi}{L}|\mathbf{n}_q|, \mathbf{n}_q \in \mathbb{Z}^3$, and definite total momentum, $|\mathbf{p}_i + \mathbf{p}_j| = \frac{2\pi}{L}|\mathbf{n}_k|, \mathbf{n}_k \in \mathbb{Z}^3$. This operator will strongly overlap with the state having invariant mass of the isobar pair (ij), $E_{ij} \simeq 2\sqrt{m^2 + (\frac{2\pi}{L}\mathbf{n}_q)^2}$, and the total energy of the three-particle system $E \simeq \sqrt{m^2 + (\frac{2\pi}{L}\mathbf{n}_k)^2} + \sqrt{E_{ij}^2 + (\frac{2\pi}{L}\mathbf{n}_k)^2}$ with small shifts caused by the interaction. Additionally, in the case of isobar dominance, fermion bilinear operators subduced from spin S_{ij} are likely to have good overlap.

VI. SUMMARY

Using the Hamlitonian formalism applied to a model of interacting relativistic fields, we derived a generalized Lüscher's formula [8, 9, 14, 15] for two-particle scattering, in both the single- and coupled-channel systems, in moving frames.

Our results are consistent with the ones obtained previously in [8, 9, 14, 15]. In the coupled-channel case we are challenged by the fact that, even for dominance of a single partial-wave, the system is underconstrained for determination of multiple-channel phase-shifts and inelasticities from a single determined finite-volume energy level. Using a toy model of two-channel S-wave scattering we demonstrated that it is possible to determine this information if multiple energy levels are determined.

Two possible strategies for extracting information from discrete spectra of a coupled-channel system were discussed, one approach utilizes the near degeneracy of energy levels in different volumes and total momenta of system, and another fits the discrete spectra by parameterizating the scattering amplitudes with certain numbers of parameters. These strategies may be useful for the analysis of future lattice QCD data. In particular, the coupled-channel analysis has to be considered for the strongly coupled systems, for instance, $\pi\pi, K\bar{K}$ and $\eta\eta$ system in S-wave.

For the case of three relativisitic particles undergoing scattering, we considered in finite-volume the isobar model approximation, where quasi-two-body scattering is assumed to be dominant. Under the isobar model approximation, the three-particle partial wave scattering amplitudes can be factorized as the product of two individual scattering amplitudes, one describes the scattering of two particles inside isobar pair, and another describes the scattering between isobar pair and the spectator particle. Three determinantal conditions, Eq. (24), (25) and (26), were obtained for three-particle scattering in a finite volume. One condition, Eq. (24), relates the scattering phase shifts of two particles inside an isobar pair to the invariant mass of the isobar pair. The other two conditions, Eqs. (25) and (26), relate the scattering phase-shifts between an isobar pair and the spectator to the total energy of the three-particle system. A proposal for extracting the phase-shifts of a three-particle system from lattice QCD simulations is presented that makes use of carefully constructed two-particle operators within the overall three-particle operator construction.

The finite volume representation of the isobar model may be suitable for systems with a sharp two-body resonance. For example, in the J/ψ to 3π decay [38], the Dalitz distribution of the 3π shows strong bands from the ρ resonance in the sub-two-pion system, such that the decaying process is well described by an isobar approximation. The rescattering effect among the three particles is expected to be negligible.

VII. ACKNOWLEDGMENTS

We thank D. B. Renner and M. R. Pennington for useful discussions, and our colleagues within the Hadron Spectrum Collaboration for their continued assistance. PG, RGE and JJD acknowledge support from U.S. Department of Energy contract DE-AC05-06OR23177, under which Jefferson Science Associates, LLC, manages and operates Jefferson Laboratory. JJD also acknowledges the support of the U.S. Department of Energy Early Career award contract de-sc0006765. APS acknowledges the support of the U.S. Department of Energy grant under contract DE-FG0287ER40365.

Appendix A: Relativistic Lippmann-Schwinger equation from Hamiltonian formalism

Following the method presented in [28, 29], we treat the relativistic dynamics of particle scattering in the Hamiltonian formalism approach. We start from the covariant Lagrangian in Eq.(1) and choose to quantize the field operators in the instant form [30]; the construction of generators of the Poincaré group can be done in a standard way in quantum field theory. In principle, one needs to solve eigenstate equations $\hat{H}|\Psi\rangle = E|\Psi\rangle$ on a instant quantization plane, where $|\Psi\rangle$ denotes the Poincaré covariant state vector spanning the complete Fock space. We truncate the Fock space up to three-body states, assuming that this is sufficient to describe low-energy physics. Thus, the eigenstate equations reduce to a matrix equation given in Eq.(2). Eliminating the three-body sector, we end up with the relativistic Schrödinger-like equation for a two-body system given in Eq.(3). For simplicity, we have assumed that the two charged scalars scattering have equal mass, however, the conclusion of this work can be trivially generalized to non-equal masses case as well (c.f. [39, 40]).

We choose the center-of-mass frame of the many-body system to construct multiple-particle states $|JM\rangle$ having total spin J and spin projection M. The two-particle state $|\phi^+\phi^-\rangle$ in the center-of-mass frame is given by

$$\big|\phi^+\phi^-; JM\big\rangle = 2\sqrt{s}\int \frac{d^3\mathbf{p}_1}{(2\pi)^3 2E_{p_1}} \frac{d^3\mathbf{p}_2}{(2\pi)^3 2E_{p_2}} \delta^3(\mathbf{p}_1+\mathbf{p}_2) \times (2\pi)^3 \varphi^{(2)}_{JM}(\mathbf{p}_1,\mathbf{p}_2)\, a^\dagger_{\mathbf{p}_1} b^\dagger_{\mathbf{p}_2}\,|0\rangle,$$

where $\mathbf{p}_i$ is the momentum of the i-th particle and $\sqrt{s}$ is the invariant mass of the two-particle system. $\varphi^{(2)}_{JM}(\mathbf{p}_1,\mathbf{p}_2)$ is the wavefunction of the two-particle system, describing the momentum distribution of the two particles.

Similarly, the three-particle state $|\phi^+\phi^-\theta\rangle$ is given by

$$\big|\phi^+\phi^-\theta; JM\big\rangle = 2\sqrt{s}\int \frac{d^3\mathbf{p}_1}{(2\pi)^3 2E_{p_1}} \frac{d^3\mathbf{p}_2}{(2\pi)^3 2E_{p_2}} \frac{d^3\mathbf{p}_3}{(2\pi)^3 2E_{p_3}} \times (2\pi)^3 \delta^3(\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_3) \times \varphi^{(3)}_{JM}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3)\, a^\dagger_{\mathbf{p}_1} b^\dagger_{\mathbf{p}_2} d^\dagger_{\mathbf{p}_3}\big|0\big\rangle,$$

where $\varphi^{(3)}_{JM}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3)$ is the wavefunction of the three-particle system. The wavefunctions are normalized so that the normalization of states is $\langle JM|JM\rangle = 2\sqrt{s}\,(2\pi)^3\,\delta^3(\mathbf{0})$.

It is straightforward to evaluate the matrix elements of the eigenstate equations Eq.(2) and to get coupled equations for the wavefunctions

$$\varphi^{(2)}_{JM}(\mathbf{q}) = \frac{g}{\sqrt{s}-2\sqrt{\mathbf{q}^2+m^2}} \int \frac{d^3\mathbf{k}'}{(2\pi)^3 2\sqrt{\mathbf{k}'^2+\mu^2}} \left[\frac{\varphi^{(3)}_{JM}(\mathbf{q}+\frac{1}{2}\mathbf{k}',\mathbf{k}')}{2\sqrt{(\mathbf{q}+\mathbf{k}')^2+m^2}} + \frac{\varphi^{(3)}_{JM}(\mathbf{q}-\frac{1}{2}\mathbf{k}',\mathbf{k}')}{2\sqrt{(\mathbf{q}-\mathbf{k}')^2+m^2}} \right],$$

$$\varphi^{(3)}_{JM}(\mathbf{q},\mathbf{k}) = g\, \frac{\frac{1}{2\sqrt{(\frac{1}{2}\mathbf{k}-\mathbf{q})^2+m^2}}\,\varphi^{(2)}_{JM}(\mathbf{q}-\frac{1}{2}\mathbf{k}) + \frac{1}{2\sqrt{(\frac{1}{2}\mathbf{k}+\mathbf{q})^2+m^2}}\,\varphi^{(2)}_{JM}(\mathbf{q}+\frac{1}{2}\mathbf{k})}{\sqrt{s}-\sqrt{(\frac{1}{2}\mathbf{k}+\mathbf{q})^2+m^2}-\sqrt{(\frac{1}{2}\mathbf{k}-\mathbf{q})^2+m^2}-\sqrt{\mathbf{k}^2+\mu^2}},$$

where we have used a short-hand notation for wavefunctions $\varphi^{(2)}_{JM}(\mathbf{q})$ and $\varphi^{(3)}_{JM}(\mathbf{q},\mathbf{k})$, with arguments of relative momenta defined by $\mathbf{q} = \frac{1}{2}(\mathbf{p}_1-\mathbf{p}_2), \mathbf{k} = -\mathbf{p}_3$. Eliminating the three-body wavefunction, we get a relativistic equation for the two-particle state $|\phi^+\phi^-\rangle$ with an effective non-local potential generated from the neutral scalar exchange between two charged scalars

$$\varphi^{(2)}_{JM}(\mathbf{q}) = \frac{1}{\sqrt{s}-2\sqrt{\mathbf{q}^2+m^2}} \int \frac{d^3\mathbf{k}}{(2\pi)^3}\, V(\mathbf{q},\mathbf{k})\,\varphi^{(2)}_{JM}(\mathbf{k}),$$

with

$$V(\mathbf{q},\mathbf{k}) = \frac{g^2}{4} \frac{1}{1-\Sigma(\mathbf{q})} \frac{1}{(\mathbf{k}^2+m^2)} \frac{1}{\sqrt{(\mathbf{k}-\mathbf{q})^2+\mu^2}} \frac{1}{\sqrt{s}-\sqrt{\mathbf{k}^2+m^2}-\sqrt{\mathbf{q}^2+m^2}-\sqrt{(\mathbf{k}-\mathbf{q})^2+\mu^2}}, \tag{A1}$$

where the self-energy contribution is,

$$\Sigma(\mathbf{q}) = \frac{1}{\sqrt{s} - 2\sqrt{\mathbf{q}^2 + m^2}} \frac{g^2}{4} \int \frac{d^3\mathbf{k}'}{(2\pi)^3} \frac{1}{\sqrt{s} - \sqrt{\mathbf{k}'^2 + m^2} - \sqrt{\mathbf{q}^2 + m^2} - \sqrt{(\mathbf{k}' - \mathbf{q})^2 + \mu^2}} \times \frac{1}{\sqrt{\mathbf{q}^2 + m^2}} \frac{1}{\sqrt{\mathbf{k}'^2 + m^2}} \frac{1}{\sqrt{(\mathbf{k}' - \mathbf{q})^2 + \mu^2}}.$$

In coordinate space, the wave-equation becomes

$$\psi_{JM}(\mathbf{r}) = \int d^3\mathbf{r}'\, G_0(\mathbf{r} - \mathbf{r}', \sqrt{s}) \int d^3\mathbf{z}\, \widetilde{V}(\mathbf{r}', -\mathbf{z})\, \psi_{JM}(\mathbf{z}),$$

where $\psi_{JM}(\mathbf{r})$ and $\widetilde{V}(\mathbf{r}', -\mathbf{z})$ are the Fourier transforms of the momentum-space two-particle wavefunction and effective potential, respectively. The free Green's function is given in Eq.(8). Performing the angular integral, the free Green's function reads

$$G_0(\mathbf{r}, \sqrt{s}) = \frac{1}{2ir} \int_{-\infty}^{\infty} \frac{q dq}{(2\pi)^2} \frac{e^{iqr} - e^{-iqr}}{\sqrt{s} - 2\sqrt{q^2 + m^2}}, \qquad \text{(A2)}$$

which has the following singularities in the complex q plane: two poles on the real axis, $q = \pm k$, and two branch cuts on the imaginary axis $\pm [im, i\infty]$, see Fig.7. We choose the contour $C_1 + C_2$ to include the pole at $q = k$ and circle around the cut $[im, i\infty]$ on the upper half-plane for first term with factor e^{ikr} and choose the contour $C_1 + C_3$ to include the pole at $q = -k$ and circle around the cut $[-im, -i\infty]$ on the lower half-plane for the second term with factor e^{-ikr}, as shown in Fig.7. The contour integral leads to

$$G_0(\mathbf{r}, \sqrt{s}) = -\frac{\sqrt{s}}{2} \frac{e^{ikr}}{4\pi r} - \frac{1}{r} \int_{m}^{\infty} \frac{\rho d\rho}{(2\pi)^2} \sqrt{\rho^2 - m^2} \frac{e^{-\rho r}}{k^2 + \rho^2},$$

where $k = \frac{1}{2}\sqrt{s - 4m^2}$ is the momentum of either particle in the rest frame of the two-particle system. The first term on the right hand side comes from the poles at $q = \pm k$ and is proportional to the usual non-relativistic Green's function which oscillates over the path of propagation. The second term comes from the contribution of the discontinuity crossing the branch cuts at $\pm [im, i\infty]$ - it decays exponentially over the propagation. Expanding $\sqrt{\rho^2 - m^2} = \rho\left(1 - \mathcal{O}\left(\frac{m^2}{\rho^2}\right)\right)$, at large separations, the free Green's function may be approximated by

$$G_0(\mathbf{r}; \sqrt{s}) \approx -\frac{\sqrt{s}}{2} \frac{1}{4\pi r} \left[e^{ikr} + \frac{2}{\pi} \frac{e^{-mr}}{r\sqrt{s}} \right], \qquad \text{(A3)}$$

and therefore the exponential decaying term can be dropped in the limit $r \gg m^{-1}$.

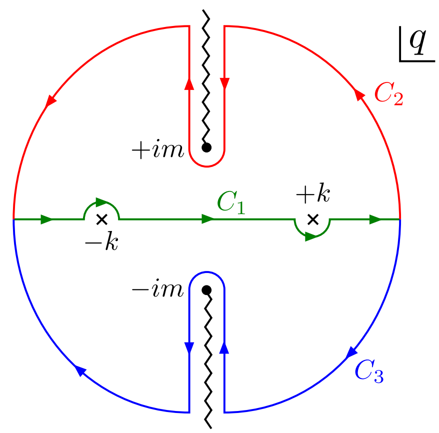

FIG. 7: Integration contours and singularities of the free Green's function in Eq.(A2) on the complex q plane.

Appendix B: Expansion of Green's function and regularization of expansion coefficients

We start from the expansion of the Green's function

$$\frac{1}{L^3} \sum_{\mathbf{q} \in \mathbf{P_Q}} \frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{k^2 - \mathbf{q}^2} = \frac{k}{4\pi}\, n_0(kr) - \sum_{jm_j} g^{(\mathbf{Q})}_{jm_j}(k)\, j_j(kr)\, Y_{jm_j}(\hat{\mathbf{r}}),$$

where the summation of $\mathbf{q}$ runs over $\mathbf{P_Q} = \{\mathbf{q} \in \mathbb{R}^3 | \mathbf{q} = \frac{2\pi}{L}\mathbf{n} + \mathbf{Q},$ for $\mathbf{n} \in \mathbb{Z}^3\}$. The expansion coefficients are given by [8]

$$g^{(\mathbf{Q})}_{jm_j}(k) = \frac{4\pi}{L^3} \sum_{\mathbf{q} \in \mathbf{P_Q}} i^j \frac{q^j}{k^j} \frac{Y^*_{jm_j}(\hat{\mathbf{q}})}{\mathbf{q}^2 - k^2} - \frac{\delta_{j0}\, \delta_{m_j 0}}{\sqrt{4\pi}} \left.\frac{1}{r}\right|_{r \to 0}. \qquad \text{(B1)}$$

Note that the definition of $n_j(x)$ in this work differs from the definition in [8] by a overall negative sign.

Using the identities

$$j_j(k|\mathbf{r} - \mathbf{r}'|)\, Y_{jm_j}(\widehat{\mathbf{r} - \mathbf{r}'}) \overset{r' \le r}{=} \sqrt{4\pi} \sum_{\substack{lm_l \\ l'm_{l'}}} i^{l - l' - j}\, j_l(kr)\, j_{l'}(kr')\, Y_{lm_l}(\hat{\mathbf{r}})\, Y^*_{l'm_{l'}}(\hat{\mathbf{r}}') \times \sqrt{\tfrac{(2j+1)(2l'+1)}{2l+1}}\, \langle jm_j; l'm_{l'} | lm_l \rangle\, \langle j0; l'0 | l0 \rangle,$$

and

$$\frac{k}{4\pi}\, n_0\big(k|\mathbf{r}-\mathbf{r}'|\big) \stackrel{r'\leq r}{=} k\sum_{lm_l} n_l(kr)\, j_l(kr')\, Y_{lm_l}(\hat{\mathbf{r}})\, Y^*_{lm_l}(\hat{\mathbf{r}}'),$$

we also have

$$\begin{aligned}\frac{1}{L^3}\sum_{\mathbf{q}\in\mathbf{P_Q}} &\frac{e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}}{k^2-\mathbf{q}^2} \\ &\stackrel{r'\leq r}{=} \sum_{\substack{lm_l\\ l'm_{l'}}} \left[\delta_{l'm'_{l'},lm_l}\, n_l(kr) - \mathcal{M}^{(\mathbf{Q})}_{l'm'_{l'},lm_l}(k)\, j_l(kr)\right], \\ &\qquad \times k\, j_{l'}(kr')\, Y_{lm_l}(\hat{\mathbf{r}})\, Y^*_{l'm_{l'}}(\hat{\mathbf{r}}'),\end{aligned} \tag{B2}$$

with

$$\begin{aligned}\mathcal{M}^{(\mathbf{Q})}_{l'm'_{l'},lm_l}(k) &= \sum_{jm_j} i^{l-l'-j}\,\frac{\sqrt{4\pi}}{k}\, g^{(\mathbf{Q})}_{jm_j}(k) \\ &\times \sqrt{\tfrac{(2j+1)(2l'+1)}{2l+1}}\,\langle jm_j; l'm_{l'}|lm_l\rangle\langle j0;l'0|l0\rangle.\end{aligned} \tag{B3}$$

If $\mathbf{Q}$ is identified with $\frac{1}{2\gamma}\mathbf{P}$ for two-particle scattering and $\frac{1}{3\gamma}\mathbf{P}$ for three-particle scattering, these expressions are the same as those presented in [9], and the regularisation procedure outlined therein can be followed.

[1] C. Michael, Nucl. Phys. B **259**, 58 (1985).
[2] M. Luscher and U. Wolff, Nucl. Phys. B **339**, 222 (1990).
[3] B. Blossier, M. Della Morte, G. von Hippel, T. Mendes and R. Sommer, JHEP **0904**, 094 (2009)
[4] J. J. Dudek *et al.* (Hadron Spectrum Collaboration), Phys. Rev. D **82**, 034508 (2010).
[5] R. G. Edwards, J. J. Dudek, D. G. Richards, and S. J. Wallace, Phys. Rev. D **84**, 074508 (2011).
[6] J. J. Dudek *et al.* (Hadron Spectrum Collaboration), Phys. Rev. D **86**, 034031 (2012).
[7] L. Maiani and M. Testa, Phys. Lett. B **245**, 585 (1990).
[8] M. Lüscher, Nucl. Phys. B **354**, 531 (1991).
[9] K. Rummukainen, S. Gottlieb, Nucl. Phys. B **450**, 397 (1995).
[10] C.-J.D. Lin, G. Martinelli, C. T. Sachrajda and M. Testa, Nucl. Phys. B **619**, 467 (2001).
[11] N. H. Christ, C. Kim and T.Yamazaki, Phys. Rev. D **72**, 114506 (2005).
[12] V. Bernard, Ulf-G. Meißner and A. Rusetsky, Nucl. Phys. B **788**, 1 (2008).
[13] V. Bernard, M. Lage, Ulf-G. Meißner and A.Rusetsky, JHEP **0808**, 024 (2008).
[14] S. He, X. Feng, C. Liu, JHEP **0507**, 011 (2005).
[15] M. Döring, Ulf-G. Meißner,E. Oset and A. Rusetsky, Eur. Phys. J. A **47**, 139 (2011)
[16] S. Aoki *et al.* [HAL QCD Collaboration], Proc. Japan Acad. B **87**, 509 (2011)
[17] R. A. Briceno and Z. Davoudi, arXiv:1204.1110 [hep-lat].
[18] M. T. Hansen and S. R. Sharpe, Phys. Rev. D **86**, 016007 (2012)
[19] S. Aoki *et al.* [CP-PACS Collaboration], Phys. Rev. D **76**, 094506 (2007)
[20] K. Sasaki, and N. Ishizuka, Phys. Rev. D **78**, 014511 (2008).
[21] X. Feng, K. Jansen, and D. B. Renner, Phys. Rev. D **83**, 094505 (2011).
[22] J. J. Dudek *et al.* (Hadron Spectrum Collaboration), Phys. Rev. D **83**, 071504 (2011).
[23] S. R. Beane *et al.* (NPLQCD Collaboration), Phys. Rev. D **85**, 034505 (2012).
[24] C. B. Lang, D. Mohler, S. Prelovsek and M. Vidmar, Phys. Rev. D **84**, 054503 (2011).
[25] S. Aoki *et al.* [CS Collaboration], Phys. Rev. D **84**, 094505 (2011)
[26] Y. Goradia and T. A. Lasinski, Phys. Rev. D **15**, 220 (1977).
[27] G. Ascoli and H. W. Wyld, Phys. Rev. D **12**, 43 (1975).
[28] S. Głazek, A. Harindranath, S. Pinsky, J. Shigemitsu, and K. Wilson, Phys. Rev. D **47**, 1599 (1993).
[29] B.L.G. Bakker, M. van Iersel, F. Pijlman, Few Body Syst. **33**, 27 (2003).
[30] P. A. M. Dirac, Rev. Mod. Phys. **21**, 392 (1949).
[31] C. E. Thomas, R. G. Edwards and J. J. Dudek, Phys. Rev. D **85**, 014507 (2012).
[32] J. L. Basdevant and E. L. Berger, Phys. Rev. D **16**, 657 (1977).
[33] L. D. Faddeev, *Mathematical Aspects of the Three-Body Problem in the Quantum Scattering Theory* (Israel Program for Scientific Translation, Jerusalem, Israel, 1965).
[34] L. D. Faddeev, Zh. Eksp. Teor. Fiz. **39**, 1459 (1960) [Sov. Phys.-JETP **12**, 1014(1961)].
[35] K. Polejaeva and A. Rusetsky, Eur. Phys. J. A**48**, 67 (2012).
[36] R. C. Hwa, Phys. Rev. **130**, 2580 (1963).
[37] R. Aaron and R. D. Amado, Phys. Rev. Lett. **31**, 1157 (1973).
[38] J. Z. Bai *et al.* (BES Collaboration), Phys. Rev. D **70**, 012005 (2004).
[39] Z. Fu , Phys. Rev. D **85**, 014506 (2012).
[40] L. Leskovec and S. Prelovsek, Phys. Rev. D **85**, 114507 (2012).